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13. ABSTRACT *(Maximum 200 words)*

Research on inorganic materials is facilitated by identifying the common features such as theoretical treatments of structure-property relationships and experimental techniques applicable to a wide range of materials. This conference helps to disseminate knowledge of such approaches and to inform scientists of common problems and interests.

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Program

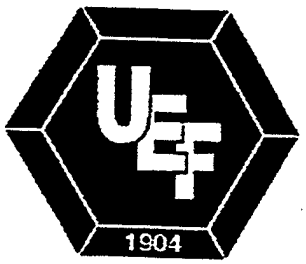
Third International Alloy Conference (IAC-3)

An Interdisciplinary Approach to the Science of Alloys in Metals, Minerals and Other Materials Systems

June 30 – July 5, 2002

Hotel Estoril Sol
Estoril /Cascais (near Lisbon), Portugal

Conference Co-Chairs:
A. Gonis, A. Meike, and P.E.A. Turchi
Lawrence Livermore National Laboratory
K. Rajan
Renssalaer Polytechnic Institute



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The Air Force Office of Scientific Research

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The Lawrence Livermore National Laboratory

The Office of Naval Research

The Metals, Minerals and Materials Society

The United Engineering Foundation, Inc.

Sunday, June 30, 2002

2:00 pm	Participant arrival and hotel check-in
5:00 pm - 7:00 pm	Registration (Hotel Lobby)
6:00 pm – 8:00 pm	Reception (Hotel Lobby)
8:00 pm - 10:00 pm	Dinner (Restaurante)

Notes

All technical sessions will be in the Cascais Room

Please, no smoking at conference technical sessions or social functions

Lunches each day (except Wednesday when you will receive a boxed lunch) are on your own

Monday, July 1, 2002

7:00 am - 8:00 am	Breakfast Buffet (Restaurante)
8:00 am - 8:30 am	Welcome and Introductions Tony Gonis, Conference Co-Chair Norm Stoloff, UEF Technical Liaison
	Session I: Chairperson: Bernard Guy
8:30 am - 9:00 am	**COMPUTER SIMULATION OF MOLTEN AND GLASSY SILICA AND ITS MIXTURES WITH SODIUM OXIDE AND ALUMINIUM OXIDE** Kurt Binder, Johannes Gutenberg Universitat Mainz, Germany
9:00 am - 9:30 am	**PARTIAL DISORDER AND BONDING IN $A_2B_2O_7$ PYROCHLORE SOLID SOLUTIONS AS A FUNCTION OF COMPOSITION AND TEMPERATURE** Bernhardt J. Wuensch, Massachusetts Institute of Technology, USA
9:30 am - 10:00 am	**THE BEHAVIOR OF SOLID SOLUTIONS IN GEOLOGICAL TRANSPORT PROCESSES: THE QUANTIZATION OF ROCK COMPOSITION BY FLUID-ROCK INTERACTION** Bernard Guy, Ecole des Mines, France
10:00 am - 10:30 am	**CATIONIC DISORDER INFLUENCE ON *AB INITIO* PHONON MODES IN THE MgAl2O4 SPINEL** Pascal Thibaudeau, C.E.A./ Le Ripault, France
10:30 am - 11:00 am	Coffee Break (Hall/Balcony)
	Session II Chairperson: Goran Grimvall
11:00 am - 11:30 am	**TEMPERATURE-DEPENDENT PROPERTIES OF FERROMAGNETIC SEMICONDUCTORS** Joseph Kudrnovsky, Institute of Physics AS CR, Czech Republic
11:30 am – 12:00 pm	**HETEROEPITAXIAL METAL GROWTH WITH INTERMIXING: A DFT-KMC APPROACH** Rossitza Pentcheva, University of Munich, Germany
12:00 pm – 12:30 pm	**AN ATOMIC SCALE STUDY OF PHYSICAL PROPERTIES OF DELTA PLUTONIUM AND Pu: Al ALLOYS** Bruno Siberchicot, CEA/DAM-DIF, France

Monday, July 1, 2002 (continued)

12:30 pm – 1:00 pm	**TIGHT-BINDING STUDIES OF METALLIC AND SEMICONDUCTING ALLOYS** Dimitri Papaconstantopoulos, Naval Research Laboratory, USA
1:00 pm - 4:30 pm	*Ad hoc* sessions/free time
4:30 pm – 5:00 pm	Afternoon Coffee (Hall/Balcony)
	Session III Chairperson: William J. Boettinger
5:00 pm - 5:30 pm	**MICROSCOPICAL DERIVATION OF GINZBURG-LANDAU-TYPE FOR ALLOYS AND THEIR APPLICATIONS TO STUDIES OF ANITPHASE AND INTERPHASE BOUNDARIES** V. G. Vaks, RRC Kurchatov Institute, Russia
5:30 pm - 6:00 pm	**WETTING BEHAVIOR IN THE Co-Pt SYSTEM** Yann Le Bouar, CNRS/ONERA LEM, France
6:00 pm - 6:30 pm	**PHASE-FIELD SIMULATIONS ON MICROSTRUCTURE EVOLUTION IN STEELS** Janin Eiken, Access e.V., Germany
6:30 pm – 7:00 pm	**A COMPUTER MODEL OF CARBONITRIDE PRECIPITATION IN STEEL** Phillipe Maugis, IRSID – Arcelor Group, France
7:00 pm - 7:30 pm	Discussion
8:00 pm - 9:30 pm	Dinner (Restaurante)
9:30 pm – 10:30 pm	Social Hour (Lobby)

Tuesday, July 2, 2002(continued)

	Session VI: Chairperson: Tony Gonis
4:45 pm - 5:15 pm	**THE CONCENTRATION AND TEMPERATURE DEPENDENCE OF SHORT-RANGE ORDER PARAMETERS IN FCC BINARY ALLOYS** Sam Faulkner, Florida Atlantic University, USA
5:15 pm – 5:45 pm	**ALLOY THERMODYNAMICS: FROM AB INITIO TO PHENOMENOLOGY** Patrice E. A. Turchi, Lawrence Livermore National Laboratories, USA
5:45 pm – 6:15 pm	**TOWARD QUANTITATIVELY ACCURATE ALLOY THEORY: SCREENED GPM INTERACTIONS** A. V. Ruban, Technical University of Denmark, Denmark
6:15 pm – 6:45 pm	**FIRST-PRINCIPLES CALCULATIONS AND THERMODYNAMIC MODELING OF LAVES PHASES** Zi-Kui Liu, Pennsylvania State University, USA
6:45 pm – 7:15 pm	**ANOMALOUS STRUCTURAL AND ELECTRONIC PROPERTIES OF C_3P_4 SOLIDS** Y. P. Feng, National University of Singapore, Singapore
7:15 pm - 7:30 pm	Discussion
8:00 pm - 9:30 pm	Dinner (Restaurante)

Wednesday, July 3, 2002

7:00 am - 8:30 am	Breakfast (Restaurante)
	Session VII Chairperson: Patrice Turchi
8:30 am - 9:00 am	**CURRENT AND FUTURE APPLICATIONS OF CALPHAD TECHNOLOGY** Larry Kaufman, Massachusetts Institute of Technology, USA
9:00 am – 9:30 am	**CHECKING EXPERIMENTAL DATA CONSISTENCY BY MEANS OF THE CALPHAD APPROACH** Suzana Fries, Access e.V., Germany
9:30 am – 10:00 am	**A THERMODYNAMIC RE-ASSESSMENT OF THE GOLD-TIN SYSTEM** Fred Hayes, University of Manchester, United Kingdom
10:00 am – 10:30 am	**MODELLING OF PHASE SEPARATION IN IRON-BASED TERNARY ALLOYS** Yoshiyuki Saito, Waseda University, Japan
10:30 am - 11:00 am	Coffee Break (Hall/Balcony)
	Session VIII Chairperson: Alan Ardell
11:00 am – 11:30 am	**TEXTURE EVOLUTION DURING GRAIN GROWTH IN ELECTRODEPOSITED NANOCRYSTALLINE Ni-Fe ALLOYS** Yong Bum Park, Sunchon National University, Korea
11:30 am – 12:00 pm	**REJUVENATION OF DEFORMATION-INDUCED INTERGRANULAR CAVITIES BY MAGNETIC FIELD ANNEALING** Tadao Watanabe, Tohoku University, Japan
12:00 pm – 12:30 pm	**SIMULATION OF STRUCTURE AND THERMOPHYSICAL PROPERTIES OF HETEROGENEOUS CONDENSED MIXTURE** S. A. Rashkovsky, Moscow Institute of Heat Technology, Russia
12:30 pm – 1:00 pm	**COMBINATORIAL DESIGN OF ALLOYS AND MATERIALS INFORMATICS** Krishna Rajan, Rensselaer Polytechnic Institute, USA
1:15 pm	Boxed Lunch Distribution and Departure for Optional Excursion. Free time for those not going on excursion.
8:00 pm – 10:00 pm	Conference Banquet (Restaurante)

Thursday, July 4, 2002

7:00 am - 8:30 am	Breakfast (Restaurante)
	Session IX Chairperson: Vaclav Drchal
8:30 am - 9:00 am	**THERMODYNAMICS OF ALKALI-LANTHANIDE HALIDES SYSTEMS:UNDERSTANDING, AND PREDICTING THE PROPERTIES OF SUCH SYSTEMS** Marcelle Gaune-Escard, Ecole Polytechnique, France
9:00 am – 9:30 am	**ORIGINS OF NON-STOICHIOMETRY AND VACANCY ORDERING IN TITANIUM CARBIDE** Barry M. Klein, University of California, USA
9:30 am – 10:00 am	***AB INITIO* STUDY OF VACANCY ORDERING IN TiC_x** P. A. Korzhavyi, Royal Institute of Technology (KTH), Sweden
10:00 am – 10:30 am	**CHARGE TRANSFER AND STRAIN EFFECTS IN DISORDERED ALLOYS** Vaclav Drchal, Institute of Physics AS CR, Czech Republic
10:30 am - 11:00 am	Coffee Break (Hall/Balcony)
	Session X Chairperson: Sam Faulkner
11:00 am - 11:30 am	**ELECTRONIC PROPERTIES OF RANDOM ALLOYS: THE EMTO-CPA THEORY** Igor Abrikosov, Uppsala University, Sweden
11:30 am – 12:00 pm	**CHARGE TRANSFERS IN METALLIC ALLOYS: A CHARGE EXCESS FUNCTIONAL THEORY** E. Bruno, University of Messina, Italy
12:00 pm – 12:30 pm	**ON THE DEVELOPMENT OF ALLOY THEORY** A. Gonis, Lawrence Livermore National Laboratories, USA
12:30 pm - 4:30 pm	*Ad hoc* sessions/free time
4:30 pm – 5:00 pm	Afternoon Coffee (Hall/Balcony)

Thursday, July 4, 2002 (continued)

Session XI
Chairperson: Suzana Fries

5:00 pm - 5:30 pm

DEPENDENCE OF ELASTIC CONSTANTS ON ALLOY COMPOSITION
Goran Grimvall, Royal Institute of Technology (KTH-SCFAB), Sweden

5:30 pm – 6:00 pm

THEORETICAL STRENGTH, MAGNETISM AND STABILITY OF INTERMETALLIC COMPOUNDS
Mojmir Sob, Institute of Physics of Materials AS CR, Czech Republic

6:00 pm – 6:30 pm

FIRST-PRINCIPLES CALCULATION OF $L1_0$-DISORDER PHASE DIAGRAM FOR Fe-Pd AND Fe-Pt SYSTEMS
Ying Chen, RACE – University of Tokyo, Japan

6:30 pm – 7:00 pm

ELASTIC ADSORBATE-ADSORBATE INTERACTIONS MEDIATED BY SUBSTRATE DEFORMATIONS
Alain Pasturel, CNRS, France

7:00 pm - 7:30 pm

Discussion

8:00 pm - 9:30 pm

Dinner (Restaurante)

Friday, July 5, 2002

7:00 am - 8:30 am	Breakfast (Restaurante)
	Session XII Chairperson: Alphonse Finel
8:30 am – 9:00 am	**STATISTICAL-THERMODYNAMIC DESCRIPTION OF THE ALLOYS WITHIN THE RING APPROXIMATION** R. V. Chepulskii, National Academy of Sciences, Ukraine
9:00 am – 9:30 am	**STUDY OF STRUCTURAL PHASE TRANSFORMATION AND PHASE STABILITY OF HCP METALS BY STATISTICAL MOMENT AND CLUSTER VARIATION METHODS** K. Masuda-Jindo, Tokyo Institute of Technology, Japan
9:30 am – 10:00 am	**ORDERING PROCESS ANALYZED BY PHASE FIELD METHOD, CVM AND PPM** Tetsuo Mohri, Hokkaido University, Japan
10:00 am – 10:30 am	**MONTE CARLO STUDY OF THE PRECIPITATION KINETICS OF Al_3Zr IN Al** Emmanuel Clouet, Pechiney, Centre de Recherches de Voreppe, France
10:30 am – 11:00 am	Coffee Break (Hall/Balcony)
	Session XIII Chairperson: Annemarie Meike
11:00 am – 11:30 am	**DEPOSITION OF HARD ALUMINA-BASED DISPERSED DIAMONDS COMPOSITE COATINGS** S. Yerakhavets, NAMATEX Systems Division, Belarus
11:30 am – 12:00 pm	**MICROSCOPICAL THEORY OF THE BIMETALLIC INTERFACE: ADHESION ENERGY OF THE SPHERICAL INCLUSION AND MATRIX** S. D. Kaim, Odessa National University, Ukraine
12:00 pm - 12:30 pm	**TRIBOLOGICAL PARAMETERS OF DEPOSITED MoS_2 AND MoS_2-ALUMINA COATINGS** M. Kireitseu, NAMATEX Systems Division, Belarus
12:30 pm - 1:00 pm	**MECHANICAL PROPERTIES OF ALUMINA-BASED COMPOSITES HARDENED BY CrC AND DIAMONDS** M. Istomin, NAMATEX Systems Division, Belarus
1:30 pm	Discussion and close of conference

POSTERS

INVESTIGATION INTO REGULARITY IN BINARY SYSTEMS BY USING "PAULING FILE BINARIES"
Ying Chen, RACE – University of Tokyo, Japan

PSEUDOPOTENTIAL THEORY OF THE SURFACE ENERGY AND TENSION OF THE LIQUID METALLIC ALLOYS
S.D.Kaim, Odessa National University, Ukraine

MANYPARTICLE INTERACTIONS IN METALLIC SYSTEMS AND SPONTANEOUS GENERATION OF INHOMOGENEOUS STATES
S.D.Kaim, Odessa National University, Ukraine

CHANGES OF LRO IN ANISOTROPIC $L1_0$-ORDERED FePd
W. Pfeiler, University of Vienna, Austria

CHARGE TRANSFERS IN METALLIC ALLOYS: A CPA THEORY
Leon Zingales, University of Messina, Italy

DETERMINATION OF THE CRITICAL NUCLEUS SIZE OF PRECIPITATES
Toru Miyazaki, Nagoya Institute of Technology

TEXTURE EVOLUTION DURING GRAIN GROWTH IN ELECTRODEPOSITED NANOCRYSTALLINE NI-FE ALLOYS
Yong Bum Park, Department of Materials Science and Metallurgical Engineering
Sunchon National University, Sunchon, Chonnam, 540-742, Korea

COMPUTER SIMULATION OF MOLTEN AND GLASSY SILICA AND ITS MIXTURES WITH SODIUM OXIDE AND ALUMINIUM OXIDE
Kurt Binder, Institut für Physik, Johannes Gutenberg Universität Mainz
Staudinger Weg 7, Mainz, 55099, Germany

PHASE DISTRIBUTION AND TRANSFORMATION DYNAMICS USING IN-SITU SYNCHROTRON DIFFRACTION METHODS
Joe Wong, Lawrence Livermore National Laboratory
PO Box 808, L-356, Livermore, CA, 94551, USA

A COMPUTER MODEL OF CARBONITRIDE PRECIPITATION IN STEEL
P. Maugis, IRSID - Arcelor Group
Voie Romaine - BP 30320, Maizières-lès-Metz, F, 57283, France

THEORETICAL STRENGTH, MAGNETISM AND STABILITY OF INTERMETALLIC COMPOUNDS
M. Sob, Institute of Physics of Materials, Acad. Sci. of the Czech Republic
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PHASE FIELD METHOD AND DISLOCATIONS.
Alphonse Finel, LEM (ONERA-CNRS)
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ORIGINS OF NON-STOICHIOMETRY AND VACANCY ORDERING IN TITANIUM CARBIDE
Barry M. Klein, University of California

DEPOSITION OF HARD ALUMINA-BASED DISPERSED DIAMONDS COMPOSITE COATINGS
S. Yerakhavets, NAMATEX System Division, Institute of Machine Reliability (INDMASH)
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TRIBOLOGICAL PARAMETERS OF DEPOSITED MOS2 AND MOS2-ALUMINA COATINGS
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MECHANICAL PROPERTIES OF ALUMINA-BASED COMPOSITES HARDENED BY CRC AND DIAMONDS
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STATISTICAL-THERMODYNAMIC DESCRIPTION OF THE ALLOYS WITHIN THE RING APPROXIMATION
R. V. Chepulskii, Department of Solid State Theory, Institute for Metal Physics
36 Vernadsky blvd., Kyiv-142, UA-03680, Ukraine

DEPENDENCE OF ORDERING PROCESS IN NI-BASED 1 1/2 0 ALLOYS ON ALLOYING ELEMENTS
S. Hata, Interdisciplinary Graduate School of Engineering Sciences, Kyushu University
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CHANGES OF LRO IN ANISOTROPIC $L1_0$-ORDERED FEPD

W. Pfeiler, Institut für Materialphysik, University of Vienna
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VACANCY-MEDIATED PHASE TRANSFORMATIONS: HOMOGENEOUS OR HETEROGENEOUS?
W. Pfeiler, Institut für Materialphysik
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CHARGE TRANSFER AND STRAIN EFFECTS IN DISORDERED ALLOYS
Vaclav Drchal, Institute of Physics AS CR
Na Slovance 2, Praha 8, none, CZ-182 21, Czech Republic

MICROSCOPICAL THEORY OF THE BIMETALLIC INTERFACE: ADHESION ENERGY OF THE SPHERICAL INCLUSION AND MATRIX
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TEMPERATURE-DEPENDENT PROPERTIES OF FERROMAGNETIC SEMICONDUCTORS
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MICROSCOPICAL THEORY OF THE BIMETALLIC INTERFACE THERMODYNAMIC PROPERTIES: ADHESION ENERGY AND INTERFACIAL TENSION OF TWO LIQUID METALS
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PSEUDOPOTENTIAL THEORY OF THE SURFACE ENERGY AND TENSION OF THE LIQUID METALLIC ALLOYS
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MANYPARTICLE INTERACTIONS IN METALLIC SYSTEMS AND SPONTANEOUS GENERATION OF INHOMOGENEOUS STATES
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A DIFFUSION MOBILITY DATABASE FOR NI-BASE SUPERALLOYS
William J. Boettinger, Metallurgy Division; NIST
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ORDERING PROCESS ANALYZED BY PHASE FIELD METHOD, CVM AND PPM
Tetsuo MOHRI, Graduate School of Engineering, Hokkaido University
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FIRST-PRINCIPLES CALCULATION OF L10-DISORDER PHASE DIAGRAM FOR FE-PD AND FE-PT SYSTEMS
Ying CHEN, RACE, University of Tokyo
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MODELLING OF PHASE SEPARATION IN IRON-BASED TERNARY ALLOYS
Yoshiyuki Saito, Waseda University
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INVESTIGATION INTO REGULARITY IN BINARY SYSTEMS BY USING "PAULING FILE BINARIES"
Ying CHEN, Research into Artifacts, Center for Engineering (RACE), University of Tokyo
Komaba 4-6-1, Meguro-ku, Tokyo, 153-8904, Japan

AB INITIO STUDY OF VACANCY ORDERING IN TIC_x
P. A. Korzhavyi, Royal Institute of Technology (KTH)
Brinellvagen 23, Stockholm, Stockholm, SE-100 44, Sweden

THERMODYNAMICS OF ALKALI-LANTHANIDE HALIDES SYSTEMS:UNDERSTANDING, AND PREDICTING THE PROPERTIES OF SUCH SYSTEMS
Marcelle Gaune-Escard, Ecole Polytechnique-IUSTI-UMR 6595 CNRS
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TOWARD QUANTITATIVELY ACCURATE ALLOY THEORY: SCREENED GPM INTERACTIONS
A. V. Ruban, Technical University of Denmark
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SIMULATION OF STRUCTURE AND THERMOPHYSICAL PROPERTIES OF HETEROGENEOUS CONDENSED MIXTURE
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ELECTRONIC PROPERTIES OF RANDOM ALLOYS: THE EMTO-CPA THEORY
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,□,‰,Ž,□,",‰,□,Ž OF THE CRITICAL NUCLEUS SIZE OF PRECIPITATES IN THE EDGE OF MISCIBILITY GAP.
Toru Miyazaki, Nagoya Institute of Technology
973-223 Minamiyama, Komenoki-cho,, Nisshin,, Aichi,, 470-0111, Japan

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Bruno Siberchicot, CEA/DAM-DIF
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MONTE CARLO STUDY OF THE PRECIPITATION KINETICS OF AL_3ZR IN AL
Emmanuel Clouet, Pechiney, Centre de Recherches de Voreppe
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GINZBURG-LANDAU FUNCTIONALS AT NOT SMALL VALUES OF ORDER PARAMETERS AND THEIR APPLICATIONS TO STUDIES OF INTERPHASE BOUNDARIES IN ALLOYS
V. G. Vaks, RRC Kurchatov Institute
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STUDY OF STRUCTURAL PHASE TRANSFORMATION AND PHASE STABILITY OF HCP METALS BY STATISTICAL MOMENT AND CLUSTER VARIATION METHODS
K. Masuda-Jindo, Tokyo Institute of Technology
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MULTIPHASE-FIELD MODEL FOR MULTICOMPONENT ALLOYS COUPLED TO THERMODYNAMIC DATABASES
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PHASE-FIELD SIMULATIONS ON MICROSTRUCTURE EVOLUTION IN STEELS
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COMBINATORIAL DESIGN OF ALLOYS AND MATERIALS INFORMATICS
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THE CONCENTRATION AND TEMPERATURE DEPENDENCE OF SHORT-RANGE ORDER PARAMETERS IN FCC BINARY ALLOYS.
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QUANTUM CONDUCTANCE OF CARBON NANOTUBES
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THERMODYNAMICS OF EPSILON IRON AT HIGH PRESSURES AND TEMPERATURES
Surendra K. Saxena, Center for the Study of Matter at Extreme Conditions
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PRECIPITATION OF DISORDERED NI-X SOLID SOLUTION PHASES IN OFF-STOICHIOMETRIC ORDERED NI_3X ALLOYS
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WETTING BEHAVIOR IN THE CO-PT SYSTEM
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PHASE FIELD MICROELASTICITY MODELING OF EVOLUTION OF COMPLEX STRUCTURES IN SINGLE AND POLYCRYSTALS
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PARTIAL DISORDER AND BONDING IN $A_2B_2O_7$ PYROCHLORE SOLID SOLUTIONS AS A FUNCTION OF COMPOSITION AND TEMPERATURE
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ANOMALOUS STRUCTURAL AND ELECTRONIC PROPERTIES OF C_3P_4 SOLIDS
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A THERMODYNAMIC RE-ASSESSMENT OF THE GOLD-TIN SYSTEM
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ALLOY THERMODYNAMICS: FROM AB INITIO TO PHENOMENOLOGY
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CURRENT AND FUTURE APPLICATIONS OF CALPHAD TECHNOLOGY
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FIRST-PRINCIPLES CALCULATIONS AND THERMODYNAMIC MODELING OF LAVES PHASES
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CHECKING EXPERIMENTAL DATA CONSISTENCY BY MEANS OF THE CALPHAD APPROACH.
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CHARGE TRANSFERS IN METALLIC ALLOYS: A CPA THEORY.
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CATIONIC DISORDER INFLUENCE ON *AB INITIO* PHONON MODES IN THE MGAL2O4 SPINEL
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HETEROEPITAXIAL METAL GROWTH WITH INTERMIXING: A DFT-KMC APPROACH
Rossitza Pentcheva, Institute of Crystallography and Applied Mineralogy, University of Munich

COMPUTER SIMULATION OF MOLTEN AND GLASSY SILICA AND ITS MIXTURES WITH SODIUM OXIDE AND ALUMINIUM OXIDE

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Molecular Dynamics simulations of silicum dioxide melts and mixtures with sodium and aluminium oxide are presented, and the static properties of these systems are analyzed, studying coordination numbers, partial structure factors, pair distribution functions, etc. We discuss the extent to which the tetrahedral SiO4 network is maintained in these melts and corresponding silicate glasses. Also the diffusion mechanism of the various ions is investigated [1]. Comparisons with various experimental data show good agreement and validate the (generalized) BKS-potential used for these simulations [2-4]. This potential has also been used successfully to study the alpha-beta-phase transition of crystalline quartz [5].

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HETEROEPITAXIAL METAL GROWTH WITH INTERMIXING: A DFT-KMC APPROACH

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Co on Cu(001) is a model system where growth involves substantial intermixing. This growth mode does not fit in the traditional picture of island nucleation as a result of binary collisions of adatoms on the surface and is not yet well understood. In a combined density-functional theory and kinetic Monte Carlo approach we demonstrate that exchange processes can have important consequences on the scaling behavior of island density and island morphology.

We employ DFT with the FP-LAPW method to identify the basic mechanisms of island nucleation and calculate their activation barriers. These processes include hopping of Co and Cu adatoms on the clean and stepped Cu(001)-surface as well as atomic exchange. Furthermore we investigate the nucleation potential of substitutionally adsorbed Co and its influence on the hopping barrier of adatoms on the surface. The rates of the microscopic processes obtained with DFT are plugged into a kinetic Monte-Carlo (kMC) simulation of the initial growth of Co on Cu(001). The scaling of the island density clearly deviates from the typical Arrhenius behavior and instead exhibts a *N* shape. This result was confirmed in ion-scattering [1] and STM experiments [2]. The driving mechanisms actuating this unexpected behavior are discussed.

Finally, we investigate the thermodynamic stability of a c(2x2)-surface alloy which was evidenced in STM experiments of a Co monolayer on Cu(001) annealed at 450K [3].

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AN ATOMIC SCALE STUDY OF PHYSICAL PROPERTIES OF DELTA PLUTONIUM AND Pu: Al ALLOYS

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The unusual behavior of plutonium metal is a result of plutonium location at a transition in the actinide series between 5f electrons participating in bonding vs. being localized. This peculiar position in the periodic table leads to its very special physical and chemical properties. For exemple, plutonium manifests itself in six allotropic forms before it melts and transformations to different crystal structures are accompanied by very large volume changes. In addition the thermal expansion within single-phase field is unusual: positive and very large for alpha monoclinic phase and negative for delta cubic phase. These later fcc phase is retained at room temperature by the addition of small amounts of IIIB elements like aluminium or gallium. Moreover plutonium and its alloys are very sensitive to aging phenomena. Phase stability may be modified under self-irradiation.

In this study, we present atomic-scale simulation of delta plutonium and Pu:Al alloys in the framework of ab initio calculations (LDA+U FPLMTO method) and classical molecular dynamics. Elastic constants of plutonium and solubility limit of aluminium in delta plutonium are calculated in rather good agreement with scarce experimental results. In addition, in order to study the properties of low energy a DMFT approach is discussed.

WETTING BEHAVIOR IN THE Co-Pt SYSTEM

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In the Co-Pt system, a simple cooling experiment can drive a sample ordered in the tetragonal L10 structure (CuAu type) close to the two-phase region involving L10 and the cubic L12 (Cu3Au type) structure. Using transmission electron microscopy observations, we show that the interfaces between two orientation domains in the L10 structure are decorated by the L12 structure and that the L12 variant formed during this wetting process is related to the characteristics of the orientation domains. Then we focus on the peculiar wetting process of the antiphase boundaries (APB's) in the L10 structure. Our TEM observations show that the APB's are decorated by three new layers: two L12 layers separated by a new L10 layer where the tetragonal axis is normal to that of the bulk domains.
To understand this peculiar wetting process, we study the thermodynamical properties of the [100] orientation and antiphase boundaries in the L10 structure. Calculations are done using an inhomogeneous Cluster Variation Method (CVM) in the tetrahedron-octahedron approximation. Our calculations predict the formation of the observed three new layers during the wetting by the ordered L12 structure of the non conservative [100] APB's in the L10 structure. Finally, we focus on the critical phenomena observed near the triple point where the wetting phenomenon is found very sensitive to the orientation of the interface.

A COMPUTER MODEL OF CARBONITRIDE PRECIPITATION IN STEEL

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In microalloyed low carbon steels, the precipitation of niobium with nitrogen and carbon leads to an increase in the strength of the sheet metal. This phenomenon occurs during the thermal processing of the steel: in the austenite phase, the precipitation of the carbonitrides slows down the recrystallisation kinetics, leading to smaller austenite grains; while in the ferrite phase, the occurrence of a dense distribution of precipitates allows for structural strengthening.

We have constructed a computer model of the precipitation kinetics of the carbonitrides that takes into account the composition evolution of the precipitates with time. The model computes the time evolution of each age-class of precipitates, thus constructing step by step the size distribution of the population. This procedure allows for the full coupling of the nucleation, growth and coarsening phenomena.

The model takes advantage of the fast diffusion of nitrogen and carbon compared to niobium to derive the composition, size and rate of formation of the precipitates during their nucleation. A local equilibrium condition is used at the precipitate-matrix interface to derive the growth rate of each precipitate as a function of its size and the current matrix composition. Coarsening occurs naturally on account of the Gibbs-Thomson capillarity effect. For isothermal heat treatments, the calculations show that the precipitates nucleate as almost pure niobium nitrides. They subsequently grow at the expense of solute nitrogen. When nitrogen is exhausted, the solute carbon precipitates and progressively transforms the nitrides into carbonitrides. The coarsening stage leads to a steady state size distribution of niobium carbonitrides of the equilibrium composition.

The precipitate composition, size and number computed as a function of time are compared with experimental data from chemical analysis, microscopy and thermo-electric power measurements.

DEPENDENCE OF ORDERING PROCESS IN Ni-BASED 1 1/2 0 ALLOYS ON ALLOYING ELEMENTS

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The ordering processes in fcc-based Ni-Mo and Ni-V alloys have been investigated by means of transmission electron microscopy and Monte Carlo simulation. These alloys exhibit diffuse intensity maxima at hkl = 1 1/2 0 in diffraction patterns for the short-range order (SRO) state. However, the transition process from the SRO to the long-range order (LRO) depends on the alloy system and composition. In the case of the Ni-Mo system, $D1_a$ and/or Pt_2Mo type LRO develops from the 1 1/2 0 type SRO, as reported previously. For the Ni-V system, on the other hand, $D0_{22}$ type ordering firstly occurs from the 1 1/2 0 type SRO, and $D0_{22}$ and/or Pt_2Mo type LRO then develops. These ordering processes were well reproduced by Monte Carlo simulation using the Ising model when the effective pairwise atomic interactions up to the ninth coordination shells were taken into account. The simulation suggested that (i) the 1 1/2 0 type SRO state is commonly rationalized as a mixed state of small segments of $D1_a$, $D0_{22}$ and Pt_2Mo structures; (ii) the SRO-LRO transition processes in the 1 1/2 0 alloys strongly depend on the pairwise interactions in longer distances than the fourth coordination distance, or many-body interactions which are not explicitly considered in the present simulation. The differences in the effective pairwise interaction parameters set for the Monte Carlo simulation are discussed in terms of the concentration of free-electrons in the Ni-Mo and Ni-V alloys.

PHASE DISTRIBUTION AND TRANSFORMATION DYNAMICS USING IN-SITU SYNCHROTRON DIFFRACTION METHODS

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Novel site-specific and fast diffraction techniques using synchrotron radiation have recently been developed to map the phases and their solid-state transformation in systems undergoing highly non-isothermal processes such as arc welding1-6. These are spatially-resolved x-ray diffraction (SRXRD), and time-resolved x-ray diffraction (TRXRD). AISI 1005, a plain carbon-manganese steel, is a pseudo-binary Fe-C system containing 0.05 wt% carbon. With increasing temperature, the system undergoes the following transformations: alpha(bcc)-gamma(fcc)-delta(bcc)-liquid. In this paper, the phase distribution in the heat-affected zone of this steel welds will be presented. Nature of the solidification product from the liquid pool, and chemical dynamics associated with the bcc-fcc transformation in a positive thermal gradient (heating), and the reverse fcc-bcc transformation in a negative thermal gradient (cooling) are elucidated using a TRXRD mode down to 50 ms. Profile analysis of the observed Bragg peaks yields detailed information on the microstructural evolution in real time and space. In-situ phase data of this sort will provide the much needed experimental inputs to realistic modeling of transformation kinetics in fusion welds, and to validate various kinetic models of phase transformation in non-isothermal systems in general.

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MULTIPHASE-FIELD MODEL FOR MULTICOMPONENT ALLOYS COUPLED TO THERMODYNAMIC DATABASES

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The phase-field method is a powerful tool for describing the spacial evolution of interfaces between different phases. In contrary to sharp-interface methods phase boundaries are described as a continuous transition between the phases. The phase-field equation allows the interfaces to move and to develop complex morphologies without need for front-tracking algorithms.

In multicomponent alloys a suitable description of the thermodynamic properties is very important, especially if the compostion is far from the dillute solution limit. In this case thermodynamic databases should be coupled to the phase-field code.

In this paper a multiphase-field model coupled to thermodynamic databases is presented which is able to handle multicomponent and multiphase evolution of morphology on a microscopic scale. Databases which are assessed according to the CALPHAD approach are connected online to the phase-field code using a thermodynamic software package. Multi-binary extrapolation is used to reduce calculation time and thus to make the simulation of realistic systems viable.

A unit cell approach is used to apply our phase-field model to remelting of Ni-base superalloys. Remelting conditions are locally considered as a directional solidification under high thermal gradients. From the results segregation pattern, secondary phase formation, incipient melting temperatures as well as homogenisation times and temperatures can be predicted which are important parameters for the further development of steam turbine alloys.

THE CONCENTRATION AND TEMPERATURE DEPENDENCE OF SHORT-RANGE ORDER PARAMETERS IN FCC BINARY ALLOYS

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The phase boundaries for binary substitutional alloys on a face-centered-cubic Bravais lattice calculated with the Monte Carlo method have been reported in the literature. The Warren-Cowley short-range order parameters (SROP) have not been studied extensively. The temperature dependence of the SROP for several concentrations will be shown for Ising models with attractive and repulsive nearest- and next-nearest-neighbor interactions. The results of these calculations will be used to illustrate the features of experimental SROP that are simply generic and those that might indicate special features of atomic interactions. A connection between the SROP and the Coulomb potential is also pointed out.

ANOMALOUS STRUCTURAL AND ELECTRONIC PROPERTIES OF C_3P_4 SOLIDS

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Group IV nitrides such as C_3N_4, Si_3N_4 and Ge_3N_4 are candidates for high-performance engineering materials due to their high bulk moduli and wide band gaps. However, no research has yet been done on the properties of group IV phosphides. We begin the theoretical investigation of the group IV phosphides by undertaking a computational study of the structural and electronic properties of carbon phosphide. To date, no research has been done on carbon phosphide although the possible existence of C_3P_4 has been postulated together with that of C_3N_4, previously a hypothetical material.

Hypothetical C_3P_4 can be obtained by substitution of N for P in C_3N_4. Considering the success of first-principles calculations in predicting the electronic and structural properties of C_3N_4, we have performed first-principles total energy calculations based on pseudopotential and plane-wave method on C_3P_4 to investigate the stability of various possible structures. As we are not aware of aware of any experimental data on crystalline carbon phosphide of any sort, we decided to begin with possible configurations previously suggested for C_3N_4 with N substituted by P.

Unlike C_3N_4, our calculations predict that pseudocubic-C_3P_4 is energetically favored relative to á-C_3P_4 and â-C_3P_4. The pseudocubic phase exhibits exceptional mechancal stability among the various structures considered. The pseudocubic phase has the lowest compressibility with the highest bulk modulus of 203 GPa among the possible crystal configurations. Being the structure with the highest density among the various phases considered, we do not expect any pathway for phase transition from the pseudocubic phase to other structural forms under pressure. Furthermore, band structure calculation reveals that pseudocubic-C_3P_4 is metallic within the local density approximation (LDA), with significant overlap between the valence and conduction bands. This suggests that if pseudocubic-C_3P_4 can be synthesized, it may be the first 3-D conducting crystal consisting of non-metallic elements.

CHECKING EXPERIMENTAL DATA CONSISTENCY BY MEANS OF THE CALPHAD APPROACH

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When collecting experimental data related to the Gibbs energy, and is derivatives for the phases in a given system, many contradictory information is found even after a carefull analysis and evaluation of the raw data published. As the CALPHAD method uses parametric models for the Gibbs energies of the different phases, and relies on experimental data for the determination of these model parameters, better the selected data, better the model parameters are determined which implies in more reliable extrapolations to unknown composition and temperature conditions and to metastable equilibria. As the method combines several types of experimental results, it can happen that contradictory information is only explicitly found after a first model parameter optimization. It can also happens that redundant experimental information coming from distinct but related derivatives of Gibbs energies leads to difficulties in the convergency of the least squares procedure. Both cases require external action of the assessor who takes decisions that depend very much on the his expertise. Examples will illustrate these facts.

MODELLING OF PHASE SEPARATION IN IRON-BASED TERNARY ALLOYS

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A theoretical model on the basis of the Cahn-Hillirad equation for multicomponent systems has been applied to the investigation of phase separation in Fe-X-Y ternary system, where X and Y are substitutional alloying elements and the concentration of the X element is higher than or equal to that of the Y element. Variation in the concentration of Y element at the peak positions of the X element was investigated with use of the model. From the analyses described above the asymptotic behavior of the minor element, Y, in an Fe-X-Y ternary alloy along a trajectory of a peak top of the major element, X, formed by phase separation is classified into three groups according to the sign of second @derivative of local free energy with respect to the concentrations of the X and the Y elements, f_{xy}. Group1(f_{xy} 0): The concentration of the Y element along the trajectory of the peak top of the X decreases with time. Group 2 ($f_{xy\ xy} < t_o$, f_{xy} 0, tt_0): At the initial stage, peaks of the concentration of the Y element formed at the same positions of the peaks tops of the X. Bifurcation of peaks occurs at the later stage. Numerical simulations of phase separation in Fe-Cr-Mo ternary alloys demonstrated the validity of the above prediction

REJUVENATION OF DEFORMATION-INDUCED INTERGRANULAR CAVITIES BY MAGNETIC FIELD ANNEALING

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Cavities and microcracks formed at grain boundaries can grow and connect to each other, causing intergranular fracture associated with severe brittleness of polycrystalline materials serving at high temperatures and in reactive environments. Different types of embrittlement such as creep embrittlement, oxidation embrittlement and stress corrosion cracking are always associated with intergranular fracture. Grain boundary engineering has been successfully applied to the control of different types of intergranular brittleness in polycrystalline materials by T. Watanabe and S. Tsurekawa (Acta Mater., 47(1999), 4171-4185).

Now a new type of approach to grain boundary engineering has been performed to obtain a basic knowledge of the rejuvenation of damaged polycrystalline ferromagnetic material, which contains intergranular cavities caused by high temperature deformation, by annealing in high magnetic fields up to 6T at temperature below the Curie temperature in an iron-cobalt alloy. In this work, polycrystalline specimens were deformed to a certain level of plastic strain (□□.03, 0.06, 01, 0.2) at 1023K and a strain rate of $3x10^{-4}s^{-1}$. The density of damaged specimens was determined and then the specimens were annealed in a magnetic field. It was found that intergranular cavities formed preferentially at random high energy boundaries at early stage of deformation. It was also found that the degree of rejuvenation determined by density measurements strongly depends on the level of plastic strain and the magnetic field strength. This is the first demonstration that magnetic field annealing is powerful to rejuvenate damaged polycrystalline materials with intergranular cavities. This newly developed processing method may be applicable to the rejuvenation of other damaged ferromagnetic materials.

COMBINATORIAL DESIGN OF ALLOYS AND MATERIALS INFORMATICS

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In this paper we provide a description of the use of combinatorial methods to design new alloys. Using novel processing strategies coupled with high throughput screening methods, we describe the methods by which complex alloy phase diagrams may be developed simultaneously with a mapping of physical properties. When coupled with multivariate statistics and data mining tools, one can begin to explore a vast parameter space in alloy development that can revolutionize and accelerate the pace of materials discovery. The value of such approaches when integrated into traditional computational and experimental strategies in alloy development is emphasized. The paper builds on examples of alloy development in multicomponent systems ranging from magnetic materials to multifunctional ceramics.

DEPENDENCE OF ELASTIC CONSTANTS ON ALLOY COMPOSITION

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The variation in the elastic shear constants in the fcc and bcc lattice structures of transition metals and their alloys is considered as a function of composition, i.e. as a function of the number of electrons per atom, e/a. Because the fcc and bcc structures appear as stable phases only in certain intervals of e/a, the experimental information is incomplete with respect to the variation through the 3d, 4d and 5d transition metal series. Ab initio electron structure calculations can give elastic shear constants with such an accuracy that they may fill gaps where experimental data are not available. In particular, it is common that the fcc lattice structure of an element or alloy is dynamically unstable, i.e. has a negative shear constant, when the bcc structure is the most stable phase, and vice versa. When information for such unstable phases is included, the shear constants show a very regular behavior as a function of e/a, similar to the variation in the cohesive energy difference between the fcc and bcc structures.

ELECTRONIC PROPERTIES OF RANDOM ALLOYS: THE EMTO-CPA THEORY

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Within the framework of the *exact muffin-tin orbitals* (EMTO) theory we have developed a new method to calculate the electronic structure and the total energy for random substitutional alloys. The problem of disorder is treated within the *coherent potential approximation* (CPA), and the total energy is obtained using the *full charge density* (FCD) technique.

Examples of applications of the FCD-EMTO-CPA method are presented. In particular, we show that it is suitable for determination of energy changes due to anisotropic lattice distortions in random alloys. We calculate the elastic constants of the Cu-rich fcc Cu-Zn alloys and optimize the *c/a* ratio for the hcp Zn-rich alloys. Mixing enthalpies are calculated for fcc, bcc and hcp Cu-Zn alloys in the complete concentration interval. The stability of *two different* hcp phases is discussed. Thermodynamic properties are also calculated for Fe-Cr alloys, and the effect of magnetic moment disorder on the mixing enthalpies is illuminated. The effect of high pressure on the phase stability is investigated for Fe-Si alloys. The method is also applied for a study of an effect of doping on phase stabilities of complex oxides.

CHARGE TRANSFER AND STRAIN EFFECTS IN DISORDERED ALLOYS

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We study the energetics of disordered alloys on an ab initio level using the TB-LMTO-CPA method. The charge-fluctuation energy is included within the Thomas-Fermi approximation. The elastic energy arising from size differences among the constituents is treated as a deformation energy of an effective continuous medium embedding the atoms. The theory is applied to various alloy systems such as Al-Li and Au-Cu. We find quite a good agreement with experimental data and calculations by other authors.

ORIGINS OF NON-STOICHIOMETRY AND VACANCY ORDERING IN TITANIUM CARBIDE

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While most stable compounds have fixed Daltonian ratios of their constituents (e.g., 1:1 ratio in ZnS, NaCl, GaAs), some materials exhibit significant nonstoichiometry, even at low temperatures. Perhaps the best known examples are NaCl-structure early transition-metal nitrides and carbides. One such example, TiC, exhibits this peculiar property of preferring the presence of vacancies (up to 50%) over a purely stoichiometric structure. Moreover, these vacancies order spatially in unusual structures. We consider TiC with vacancies as a binary alloy and express the energy of any of the 2^N configurations in a mixed-basis cluster expansion obtained from ab initio calculations of 30 ordered structures. A ground state search of all possible configurations reveals that, indeed, an ordered array of vacancies has the lowest energy. We show systematic features in the electronic structure that help explain the preference for vacancies.

THEORETICAL STRENGTH, MAGNETISM AND STABILITY OF INTERMETALLIC COMPOUNDS

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Theoretical strength and stability of intermetallic compouds is studied by means of first-principles electronic structure calculations. Tensile test is simulated under fully relaxed conditions and ideal tensile strength is determined for NiAl, MoSi2 and WSi2. The importance of presence or absence of higher-symmetry structures along the deformation path for the shape of the total energy profile is stressed. In Ni3Al, changes in magnetic behavior along the trigonal and tetragonal displacive phase transformation paths are investigated. Both L12 and D03 structures are considered. The interphase boundaries between the ferromagnetic and non-magnetic phases are found. The magnetic moments and elastic properties of high-symmetry structures are compared to available experimental data.

ELASTIC ADSORBATE-ADSORBATE INTERACTIONS MEDIATED BY SUBSTRATE DEFORMATIONS

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We calculate the elastic interaction energy between two oxygen atoms on a graphite basal plane surface by atomic ab initio calculations and continuum theory of elasticity. The comparison between the results obtained with the two different methods, despite their usual length scale domain of application, is very good; attractive and repulsive behaviors are found. This type of interaction could play an important role in the self-organization of oxygen atoms on a graphite surface.

ORDERING PROCESS ANALYZED BY PHASE FIELD METHOD, CVM AND PPM

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By combining Phase Field Method (PFM) with Cluster Variation Method (CVM), ordering processes associated with L10 ordered phase at a fixed 1:1 stoichiometric composition are analyzed. The emphasis is placed on the cooperative phenomenon from atomistic to microstructural scales.

For disorder-order relaxation process, Nucleation-Growth process and Spinodal Ordering process are not distinguishable in the atomistic scale. However it can be shown by a simple one-dimensional calculation that the former proceeds by the lateral motion of the ordered domain boundary while the latter is characterized by the gradual and homogeneous enhancement of Long Range Order for an entire specimen. Two-dimensional calculation is also attempted, and triple point junction of APB is reproduced when the free energy is formulated by properly considering the variants of ordered domain.

For order-order relaxation process, the present study distinguishes three kinds of relaxations; (1)atomistic, (2)wetting and (3)movement of Anti Phase Boundary. Each process is distinguished by different time constant, and (1) and (2) are well fitted in the conventional exponential function.

Path Probability Method (PPM) has been known as the natural extension of the CVM to time domain. Comparison of disorder-order transition kinetics is attempted between PPM and CVM-PFM. It is confirmed that for near-equilibrium transition, both methods trace nearly isomorphic kinetic paths on the free energy contour surface, while for far-from-equilibrium transition the deviation is emphasized.

MICROSCOPICAL THEORY OF THE BIMETALLIC INTERFACE: ADHESION ENERGY OF THE SPHERICAL INCLUSION AND MATRIX

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In framework of the manyparticle self-consistent theory and psedopoten- tial conception the expression for energy of bimetallic system of the spherical inclusion and matrix for any order of the pseudopotential perturbation theory is obtained. In second order the adhesion energy of the spherical inclusion and matrix is calculated. The adhesion energy in terms of the surface energy of spherical metal particle, surface energy of spherical void in metal matrix and "interfacial energy" of the inclusion-matrix system is expressed. The full self-consistent systems of equations for description of the electronic and ionic structures of the metallic particle, spherical void in metal matrix and for inclusion-matrix system are obtained. In second order of the pseudopotential perturbation theory the expressions for surface energy of the spherical particle, for surface energy of the spherical void in metal matrix and for "interfacial energy" of the inclusion-matrix system are obtained. For all enumeratied thermodynamic functions the pair interparticle interactions and correlations taken into account. The surface energy of the metal particle, surface energy of the spherical void in metal matrix and "interfacial energy" have size depen- dence. All results are suitable for bimetallic inclusion-matrix system in arbitrary phase state (solid, liquid, amorphous)

MECHANICAL PROPERTIES OF ALUMINA-BASED COMPOSITES HARDENED BY CrC AND DIAMONDS

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The possibility to manufacture materials with a functional gradient of mechanical properties such as hardness, toughness and wear resistance by electrophoresis have been investigated. Al2O3/CrC and Al2O3/ultra dispersed diamonds functionally graded composites were processed by electrophoretic deposition, pyrolitic deposition and pressureless sintering in air. The composites show a continuous variation in composition and microstructure. The Vickers hardness was found to increase continuously in the depth, whereas the indentation fracture toughness decreases along the same direction. In the Al2O3/CrC composite, the hardness increases from 12 to 16 GPa, whereas the toughness decreases from 3,5 to 2,7 MPa m1/2. In the Al2O3/ultra dispersed diamonds composite, the hardness increases from 12 to 19 GPa, and the toughness decreases from 3,5 to 2,9 MPa m1/2. The most challenging problems in the processing are found to be the cracking of the deposit during drying and the cracking of the sintered body during heating. At the moment, the production of small specimens without cracking is possible, but the production of large parts still remains a challenge. The solution of the cracking problem needs more laboratory experience and the support of theoretical calculations of material properties and residual thermal stresses in graded materials. From the above mentioned experiments, we can conclude that it is feasible to produce the graded tribological composite based on alumina by electrophoretic forming and pressure less sintering. A continuous gradient of composition in the composites can be produced by changing the composition of the suspension during electrophoretic deposition and is maintained after sintering.

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